

# Spin and charge inhomogeneities in high- $T_c$ cuprates: Evidence from NMR and neutron scattering experiments

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In this communication we consider the doping dependence of the strong antiferromagnetic spin fluctuations in the cuprate superconductors. We investigate the effect of an incommensurate magnetic response, as recently observed in inelastic neutron scattering (INS) experiments on several  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  compounds, on the spin-lattice and spin-echo relaxation rates measured in nuclear magnetic resonance (NMR) experiments. We conclude that a consistent theoretical description of INS and NMR can be reached if one assumes spatially inhomogeneous but locally commensurate spin correlations and that NMR and INS experiments can be described within a single theoretical scenario. We discuss a simple scenario of spin and charge inhomogeneities which includes the main physical ingredients required for consistency with experiments.

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## I. INTRODUCTION

Understanding the doping, frequency and temperature dependence of the magnetic response in the high- $T_c$  cuprates is one of the most challenging problems for the high- $T_c$  community. Insight into the nature of the strong antiferromagnetic fluctuations very likely holds the key to the unusual normal state properties of the cuprates [1,2], as seen in a variety of experimental techniques. Both nuclear magnetic resonance (NMR) and inelastic neutron scattering (INS) experiments are important tools to probe spin excitations in cuprates [3–5]. While INS experiments provide insight into the momentum and frequency resolved imaginary part of the spin susceptibility,  $\chi(\mathbf{q}, \omega)$ , NMR experiments yield information on the momentum averaged real and imaginary part of  $\chi(\mathbf{q}, \omega)$  in the zero frequency limit. However, in contrast to NMR experiments, INS measurements rely on the existence of large single crystals and often suffer from a rather limited experimental resolution. Therefore, these experimental techniques are complementary in the information provided on spin excitations in the cuprates.

One of the central questions in the cuprate superconductors is whether INS and NMR experiments can be simultaneously understood within a single theoretical scenario. Thus far it is not even been clear whether one can reach agreement between INS and NMR data as far as the order of magnitude of the spin susceptibility is concerned. This problem is caused, in part, by the fact that NMR is sensitive to all magnetic fluctuations, regardless of whether they are related to a pronounced momentum dependence of the spin susceptibility. In contrast, INS typically probes only those parts of the susceptibility which are strongly momentum dependent; the rest are typically attributed to the “background” of the signal, as might be caused by the scattering of neutrons on nuclei and phonons.

The situation has been further complicated by recent INS experiments on  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  which observe a crossover from a substantial incommensuration in the magnetic response at low frequencies, to a commensurate structure in  $\chi$  at higher frequencies [6–8]. The question thus arises: does this incommensurate order originate from spatially inhomogeneous correlations between the doped holes [9], which would preserve a locally commensurate magnetic response, or does it reflect homogeneous incommensuration, most likely due to Fermi surface effects.

In this communication we argue that since NMR experiments probe the local spin environment around a nucleus, they are able to distinguish between a locally commensurate and incommensurate magnetic response. Earlier theoretical studies of NMR experiments on  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  and  $\text{YBa}_2\text{Cu}_4\text{O}_8$  used a phenomenological form of  $\chi$  [10]:

$$\chi(\mathbf{q}, \omega) = \frac{\alpha \xi^2}{1 + \xi^2(\mathbf{q} - \mathbf{Q})^2 - i\omega/\omega_{sf}}, \quad (1)$$

where  $\xi$  is the magnetic correlation length in units of the lattice constant,  $a_0$ ,  $\omega_{sf}$  an energy scale characterizing the diffusive spin excitations,  $\alpha$  an overall temperature independent constant, and  $\mathbf{Q}$  is the position of the peak in momentum space which was assumed to be commensurate, i.e.  $\mathbf{Q} = (\pi, \pi)$ . Using this expression for  $\chi(\mathbf{q}, \omega)$  a rather detailed quantitative understanding of various NMR data has been reached [11–13]. In particular, from the analysis of the longitudinal spin lattice relaxation rate of the  $^{63}\text{Cu}$  nuclei,  $1/T_1$ , and the spin spin relaxation time,  $1/T_{2G}$ , scaling laws like  $\omega_{sf} \propto \xi^{-z}$  with dynamical critical exponent,  $z$ , have been deduced. It was found that  $z \approx 1$  between a lower crossover temperature,  $T_*$ , and a higher one,  $T_{cr}$ , whereas  $z \approx 2$  above  $T_{cr}$ . In the temperature range where  $z = 1$  scaling applies, it follows that  $T_1 T / T_{2G}$  is independent of temper-

ature; a conjecture which was experimentally verified by Curro *et al.* for  $\text{YBa}_2\text{Cu}_4\text{O}_8$  [14]. Below the pseudogap temperature,  $T_*$ ,  $\omega_{\text{sf}}$  and  $\xi$  decouple and a quasiparticle and spin pseudogap emerges. Moreover, it was recently shown that the temperature dependence of the incommensurate peak width, as determined in INS experiments on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  [15], showed  $z = 1$  scaling over a wide range of temperatures, in agreement with the NMR findings for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . Because of its appearance in both NMR and INS results, we will therefore assume in the following analysis that  $z = 1$  is the proper scaling behavior for magnetically underdoped cuprates between  $T_*$  and  $T_{\text{cr}}$ .

One of our central results is that the attempt to understand the NMR data for  $\text{YBa}_2\text{Cu}_4\text{O}_8$  with homogeneous incommensuration is inconsistent with  $z = 1$  scaling. This implies that the local magnetic response, which is probed in NMR experiments, is commensurate. Should INS experiments show that this compound exhibits a (globally) incommensurate magnetic response similar to that seen in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ , this would strongly support a dynamic charge and spin inhomogeneity (stripe) origin of the incommensuration. In Sec. V we discuss a *spin and charge inhomogeneity* scenario which reconciles the global incommensuration with the local commensuration in  $\chi$ .

In a second important result we carry out a quantitative comparison of the strength of the antiferromagnetic spin fluctuations, as measured by NMR and INS experiments. We find that agreement between the results obtained from these quite different experimental techniques, which explore not only a different frequency range, but different wavevector regimes, can be obtained within a factor of 2. Given the large uncertainties in determining the absolute value of  $\chi''$ , we believe that this result demonstrates that a consistent description of INS and NMR data can be achieved within the framework of Eq.(1).

Although the form of  $\chi$  in Eq.(1) was originally invented to understand the spin response at very low frequencies and above the superconducting transition temperature [10], it has proved interesting to investigate to what extent one can understand INS data at higher frequencies within the same framework. The results by Aeppli *et al.* support the picture of a unique incommensurate spin response from zero energy up to 15 meV, the highest energy used in Ref. [15]. Within the error bars of the experiment, only for momentum values away from the peak maximum do systematic deviations from Eq.(1) occur. Such deviations indicate the presence of lattice corrections to the continuum limit used in Eq.(1). Lattice corrections are expected to be extremely important for the local, momentum averaged, susceptibility:

$$\chi''_{\text{loc}}(\omega) = \frac{1}{4\pi^2} \int_{BZ} d^2\mathbf{q} \chi''(\mathbf{q}, \omega), \quad (2)$$

since the phase space of momenta away from the peak maxima is considerable in two dimensions. For higher

frequencies spin excitations away from the antiferromagnetic peak and energetically large compared to  $\omega_{\text{sf}}$  come into play and we therefore expect a poor description of  $\chi''_{\text{loc}}(\omega)$  in terms of Eq.(1). This conclusion is independent of whether the peak position commensurate or incommensurate peaks.

Deviations from the universal continuum limit of  $\chi$  are expected to be also of relevance for the relaxation rates measured in NMR experiments since these are weighted momentum averages of  $\chi(\mathbf{q}, \omega)$ . Thus, it is worthwhile to study whether one can find indications for lattice corrections from an analysis of NMR and INS data. Such corrections to  $\chi$  are also of relevance for our understanding of the lifetime of so-called *cold* quasiparticles if one assumes that the lifetime of these quasiparticles is also dominated by scattering off spin fluctuations [16–19].

Our paper is organized as follows. In Sec. II we give a brief overview of the theoretical framework in which we analyze the INS and NMR data. In Sec. III A we analyze NMR data on  $\text{YBa}_2\text{Cu}_4\text{O}_8$  for both commensurate and incommensurate magnetic response and discuss the role of lattice corrections. In Secs. III B and III C we analyze NMR data on two  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  compounds. In Sec. IV we discuss the consistency between NMR and INS data, as well as the role of lattice corrections for the local susceptibility. In Sec. V we propose a *spin and charge inhomogeneity* scenario as a possible way to reconcile NMR and INS data. Finally, in Sec. VI we draw our conclusions.

## II. THEORETICAL OVERVIEW

We briefly discuss the theoretical framework in which we discuss NMR and INS experiments. In order to analyze the low frequency NMR data, we use the dynamical spin susceptibility of Eq.(1), where for the commensurate case  $\mathbf{Q} = (\pi, \pi)$ . To allow for an incommensurate structure of  $\chi$ , we use Eq.(1) with  $\mathbf{Q} = (1, 1 \pm \delta)\pi$  and  $\mathbf{Q} = (1 \pm \delta, 1)\pi$  and sum over all four peaks [11]. The inclusion of the correct form of lattice corrections is rather difficult since it requires a microscopic model which is beyond the scope of this paper. In general we expect lattice corrections to appear in the form of an upper momentum cutoff,  $\Lambda$ . In the following we choose a soft cutoff procedure for  $\delta\mathbf{q} \equiv \mathbf{q} - \mathbf{Q}$  in the denominator of Eq.(1):

$$\delta\mathbf{q}^2 \rightarrow \delta\mathbf{q}^2 \left( 1 + \frac{\delta\mathbf{q}^2}{\Lambda^2} \right). \quad (3)$$

We also expect a weak momentum dependence of  $\alpha$  and  $\omega_{\text{sf}}$  once the continuum description breaks down; however, to keep the number of tunable parameters small we ignore these effects.

In NMR experiments, one measures the spin-lattice relaxation rate  $1/T_{1x}$ , with applied magnetic field in  $x$ -direction, and the spin-echo rate  $1/T_{2G}$ , which can be expressed in terms of the dynamical susceptibility as:

$$\frac{1}{T_{1x}T} = \frac{k_B}{2\hbar}(\hbar^2\gamma_n\gamma_e)^2 \frac{1}{N} \sum_q F_x(q) \lim_{\omega \rightarrow 0} \frac{\chi''(q, \omega)}{\omega}, \quad (4)$$

$$\left(\frac{1}{T_{2G}}\right)^2 = \frac{0.69}{128\hbar^2}(\hbar^2\gamma_n\gamma_e)^4 \left\{ \frac{1}{N} \sum_q \left[ F_{ab}^{eff}(q)\chi'(q, \omega) \right]^2 - \left[ \sum_q F_{ab}^{eff}(q)\chi'(q, \omega) \right]^2 \right\}, \quad (5)$$

where  $x = ab, c$  describes the direction of the external magnetic field. The  $^{63}Cu$  form factors are given by

$$^{63}F_c(q) = \left[ A_{ab} + 2B(\cos(q_x) + \cos(q_y)) \right]^2, \quad (6)$$

$$^{63}F_{ab}^{eff}(q) = \left[ A_c + 2B(\cos(q_x) + \cos(q_y)) \right]^2, \quad (7)$$

$$^{63}F_{ab}(q) = \frac{1}{2} \left[ ^{63}F_{ab}^{eff}(q) + ^{63}F_c(q) \right]. \quad (8)$$

where  $A_{ab}, A_c$  and  $B$  are the on-site and transferred hyperfine coupling constants, respectively [11].

It follows from Eq.(1) that the spin excitations in the normal state are completely described by three parameters,  $\alpha, \xi$ , and  $\omega_{sf}$ . In order to extract these parameters from the experimental NMR data, we also need to obtain the three hyperfine coupling constants,  $A_{ab}, A_c$ , and  $B$ ; hence we have six unknown parameters in the above equations, and require six equations to determine them. So far we have two, Eqs.(4) and (5). An additional constraint arises from the temperature independence of the  $^{63}Cu$  Knight shift in a magnetic field parallel to the  $c$  axis in  $YBa_2Cu_3O_7$  [11] which yields

$$A_c + 4B \approx 0. \quad (9)$$

A fourth constraint comes from the anisotropy of the  $^{63}Cu$  spin-lattice relaxation rates [20], which for  $YBa_2Cu_3O_7$  was measured to be

$$^{63}R = \frac{T_{1c}}{T_{1ab}} \approx 3.7 \pm 0.1. \quad (10)$$

A fifth constraint involving the hyperfine coupling constants can be obtained by plotting the Knight shift  $^{63}K_{ab}$  versus  $\chi_0(T)$  [11], which yields

$$4B + A_{ab} \approx 200 \frac{kOe}{\mu_B}. \quad (11)$$

A final constraint is obtained from the earlier conjecture that the antiferromagnetic correlation length at the crossover temperature  $T_{cr}$  is approximately two lattice constants [13]. Recent microscopic calculations have confirmed this conjecture, showing that indeed  $\xi(T_{cr})$  is of the order of a few lattice constants [21].

To the extent that experimental data for  $T_1$  and  $T_{2G}$  are available up to  $T_{cr}$ , one can fit the above set of

six equations self-consistently to the data, and thus obtain not only the temperature independent parameters  $\alpha, A_{ab}, A_c$ , and  $B$ , but also the temperature dependence of  $\xi$  and  $\omega_{sf}$ . It turns out, however, that this analysis is only possible for  $YBa_2Cu_4O_8$ , since this is the single compound for which data up to sufficiently high temperatures have been obtained [14]. Our corresponding results will be presented in section III A. In order to extract the relevant parameters from NMR data on the related, widely studied,  $YBa_2Cu_3O_{6+x}$  compounds, and thus to make a comparison between NMR and INS experiments possible, we need to make two assumptions, which, at least partly, will be supported by the experimental data for  $YBa_2Cu_4O_8$ . First, we assume a relation between  $\omega_{sf}$  and  $\xi$ , given by [12,13]

$$\omega_{sf} = \hat{c}\xi^{-z}, \quad (12)$$

where  $\hat{c}$  is a temperature independent constant. For  $YBa_2Cu_4O_8$ , where we can independently extract  $\omega_{sf}$  and  $\xi$ , we will show that there is indeed a crossover from  $z = 1$  behavior at low temperature to  $z = 2$  behavior at higher temperatures. The second assumption concerns the temperature dependence of the magnetic correlation length,  $\xi(T)$ , which we take to be that obtained by one of us using a renormalization group (RG) approach [22]: for  $z = 1$  the temperature dependence of the magnetic correlation length is given by

$$\xi^{-2} = \xi_0^{-2} + bT^2, \quad (13)$$

a result which is in good agreement with INS experiments on  $La_{2-x}Sr_xCuO_4$  [15]. Having all the necessary theoretical tools in place, we now address the questions raised in the introduction.

### III. ANALYSIS OF NMR EXPERIMENTS

#### A. $YBa_2Cu_4O_8$

$YBa_2Cu_4O_8$  is a benchmark system for our analysis, since Curro *et al.* [14] have measured the relaxation times  $T_1$  and  $T_{2G}$  over a wide temperature range from 80K to 750K, and in particular between  $T_* \approx 200$  K and  $T_{cr} \approx 500$  K. We are therefore able to extract the relevant parameters which we discussed above from a self-consistent fit of Eqs.(4)-(11) to the  $T_1$  and  $T_{2G}$  data. In doing so, we assume that the constraints given by Eqs.(9)-(11) for  $YBa_2Cu_3O_7$  are also valid for  $YBa_2Cu_4O_8$ . Since we can determine  $\xi$  and  $\omega_{sf}$  independently, we are able to study the effect of both an incommensurate magnetic response, and of non-universal lattice corrections, on the scaling law  $\omega_{sf} = \hat{c}/\xi^z$ .

We first reconsider the case of a commensurate structure of  $\chi$ , and set  $\Lambda = 2\sqrt{\pi}$ , i.e. we choose a momentum cut-off which corresponds to the linear size of the BZ. We present the temperature dependence of both  $\omega_{sf}$  and  $\xi^{-1}$ ,

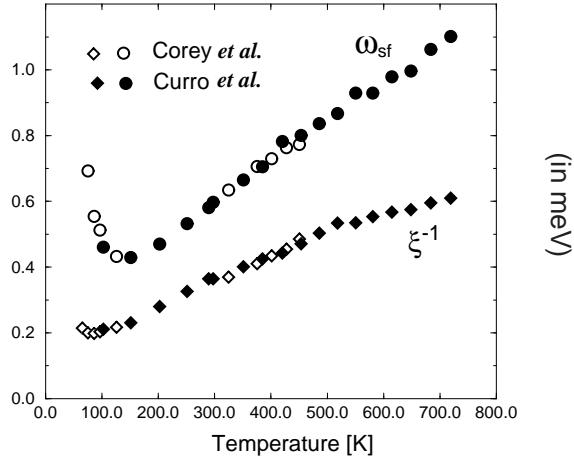


FIG. 1. The temperature dependence of  $\omega_{sf}$  and  $\xi^{-1}$  in  $\text{YBa}_2\text{Cu}_4\text{O}_8$  for the commensurate case with  $\Lambda = 2\pi^{1/2}$ .

which results from a self-consistent fit to the experimental data, in Fig. 1. Between  $T_* = 200$  K and  $T_{cr} = 500$  K,  $\omega_{sf}$  and  $\xi^{-1}$  clearly scale linearly with temperature. In order to study the extent to which  $\omega_{sf}$  and  $\xi$  obey the above scaling law, we plot in Fig. 2,  $\ln(\omega_{sf})$  as a function of  $\ln(\xi)$  (lower curve). The dynamical scaling range is of course too limited to prove the existence of a scaling relation. However, assuming  $\omega_{sf} \propto \xi^{-z}$ , we find  $z \approx 1$  below 500 K, which we identify with  $T_{cr}$  and  $z \approx 2$  above  $T_{cr}$ . These results are consistent with an earlier analysis of the scaling behavior [12,13] and the microscopic scenario of Ref. [21]. To study the effect of stronger lattice corrections, we decreased  $\Lambda$  to  $\Lambda = 2\sqrt{\pi}/4$  (upper curve in Fig. 2 which for clarity is offset). Our conclusions concerning the scaling relations remain unchanged. We can thus conclude that the dynamical scaling behavior of spin excitations is robust against even sizeable lattice corrections, as long as the structure of  $\chi''$  is commensurate.

We next examine the effect of incommensuration on the dynamical scaling. It was earlier argued that the magnetic response in  $\text{YBa}_2\text{Cu}_4\text{O}_8$  should be very similar to  $\text{YBa}_2\text{Cu}_3\text{O}_{6.8}$  [13]. Using the observed doping dependence of the incommensuration in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ , we estimate the incommensuration in  $\text{YBa}_2\text{Cu}_4\text{O}_{8+x}$  to be  $\delta = 0.23$ . Setting  $\Lambda = 2\sqrt{\pi}$  we plot in Fig. 3  $\ln(\omega_{sf})$  as a function of  $\ln(\xi)$  (lower curve) and find, following the same argumentation as above, that the dynamical scaling exponent below  $T_{cr} \approx 500$  K is now  $z \approx 0.75$ . Increasing the strength of the lattice corrections by decreasing  $\Lambda$  we find that  $z$  is increased. However, in order to obtain again  $z \approx 1$  (the upper curve in Fig. 3), which one would expect from the INS data on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ , we need a very small momentum cut-off,  $\Lambda \approx 2\sqrt{\pi}/15$ . Such a small cut-off of order  $O(1/\xi)$  is inconsistent with the continuum theory which is the basis for a dynamical scaling approach. We therefore conclude that a spatially ho-

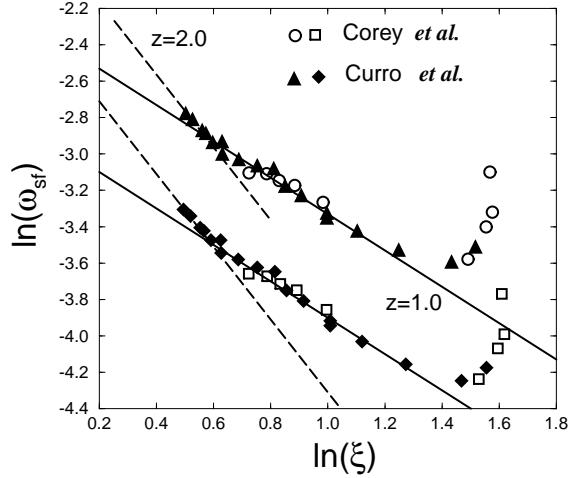


FIG. 2.  $\ln(\omega_{sf})$  as a function of  $\ln(\xi)$  for the commensurate case. Upper data set:  $\Lambda = 2\pi^{1/2}/4$ ; Lower data set:  $\Lambda = 2\pi^{1/2}$ . Solid line:  $z=1$ ; dashed line:  $z=2$ .

mogeneous incommensurate magnetic response is in contradiction with the available NMR data. The physical origin of this sensitivity of the magnetic response of a homogeneously incommensurate system, compared to a locally commensurate one, results from the fact that the former effectively decreases the spatial extent of the spin-spin correlations, thus increasing the role of large values of  $\delta\mathbf{q} \sim \Lambda$ . It should also be noted that our arguments using lattice corrections to discriminate between these two scenarios works only for intermediate values of the correlation length. For very large  $\xi$  the system should be insensitive to the cut-off procedure regardless of whether it is commensurate or incommensurate.

In what follows we assume that the low frequency magnetic response measured in an NMR experiment is indeed locally commensurate which implies that  $z = 1$  scaling prevails between  $T_*$  and  $T_{cr}$ . In Sec. V we present a possible theoretical scenario to resolve this apparent contradiction between the incommensuration seen in INS experiments and our conclusions based on the available NMR data. Finally, using the commensurate form of Eq.(1), and a momentum cut-off  $\Lambda = 2\sqrt{\pi}$  we find the following parameters from the solution of the above self-consistent equations:  $\alpha = 10\text{eV}^{-1}$ ,  $A_{ab} = 20.2\text{kOe}/\mu_B$ ,  $A_c = -182.8\text{kOe}/\mu_B$ , and  $B = 45.7\text{kOe}/\mu_B$  for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ .

## B. $\text{YBa}_2\text{Cu}_3\text{O}_7$

Since it was earlier argued that for the optimally doped  $\text{YBa}_2\text{Cu}_3\text{O}_7$ ,  $T_{cr} \approx 125$  K, only slightly above  $T_c$ , there is no significant temperature dependence of the relaxation rates between  $T_c$  and  $T_{cr}$ . We will therefore perform our analysis of the NMR data only at  $T_{cr}$ . Assuming that  $\xi(T_{cr}) = 2$ , and setting  $\Lambda = 2\sqrt{\pi}$ , we utilize  $T_{2G}$  data by Itoh *et al.* [23] and Stern *et al.* [24], as

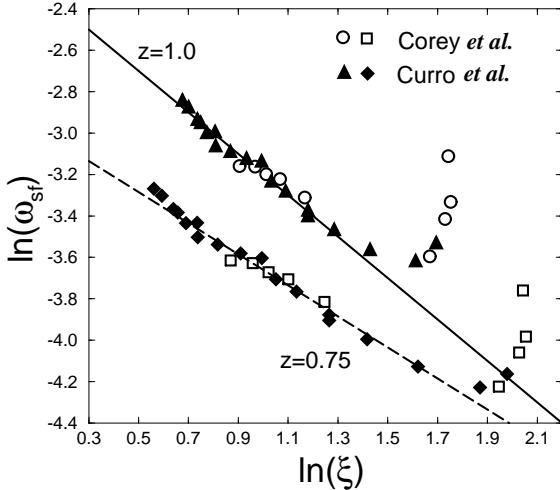


FIG. 3.  $\ln(\omega_{sf})$  as a function of  $\ln(\xi)$  for the incommensurate case. Lower data set:  $\Lambda = 2\pi^{1/2}$ ; Upper data set:  $\Lambda = 2\pi^{1/2}/15$ . Solid line:  $z=1$ ; dashed line:  $z=0.75$ .

well as  $T_{1c}$  data by Hammel *et al.* [25] to find the following hyperfine coupling constants  $A_{ab} = 27.8 \text{ kOe}/\mu_B$ ,  $A_c = -175.2 \text{ kOe}/\mu_B$ , and  $B = 43.9 \text{ kOe}/\mu_B$ . Note that these values agree well with the hyperfine coupling constants we extracted for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . With  $1/T_{2G} = 10^4 \text{ s}^{-1}$  and  $T_{1c}T \approx 0.15 \text{ Ks}$  at  $T_{cr}$ , we obtain  $\alpha = 18.5 \text{ eV}^{-1}$ ,  $\omega_{sf} \approx 19.8 \text{ meV}$  and  $\hat{c} \approx 39.6 \text{ meV}$ . It turns out that the above parameter set is rather robust against changes in  $\Lambda$ . When  $\Lambda$  is decreased from  $\Lambda = 2\sqrt{\pi}$  to  $\Lambda = 2\sqrt{\pi}/4$ ,  $A_c$  and  $B$  decrease by about 1.5%,  $A_{ab}$  increases by about 8.5%,  $\alpha$  increases by 11%, and  $\omega_{sf}$  decreases by about 15%. A change of the momentum cut-off by a factor of 4, which decreases the area of integration in the BZ by a factor of 16, thus leads only to moderate changes in the parameter set. However, as we show in Sec. IV, the corresponding changes in the local susceptibility at high frequencies are much more dramatic.

### C. $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$

In what follows we show that, though only a limited set of NMR data on  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$  is available, we nevertheless reach the same conclusions regarding the scaling behavior as in  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . In particular, since no NMR data on  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$  are available above  $T = 300 \text{ K}$ , and since we do not know the exact value of  $T_{cr}$ , we cannot extract the parameter set from a self-consistent fit to the NMR data as we did in the case of  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . However, it is in this doping range that INS data are available and therefore a consistency check between the parameter sets extracted from NMR and INS measurements might be the most promising. It turns out that though we are not able to perform a fully self-consistent fit, we can still extract the parameter set if we make sev-

	$\alpha (\text{eV}^{-1})$	$\hat{c} (\text{meV})$	$b (10^{-7} \text{ K}^2)$	$\xi_0^{-2} (10^{-2})$
$T_{cr} = 650 \text{ K}$ $\Lambda = 2\sqrt{\pi}$	11.0	68.1	5.1	3.5
$T_{cr} = 650 \text{ K}$ $\Lambda = 2\sqrt{\pi}/4$	12.2	61.2	5.0	3.9
$T_{cr} = 550 \text{ K}$ $\Lambda = 2\sqrt{\pi}$	13.0	67.3	6.7	4.7
$T_{cr} = 550 \text{ K}$ $\Lambda = 2\sqrt{\pi}/4$	14.5	59.9	6.5	5.3

TABLE I. Parameter sets for two different values of  $T_{cr}$  and  $\Lambda$ .

eral additional assumptions which are supported by our results on  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . First, we assume that  $z = 1$  scaling is present between  $T_*$  and  $T_{cr}$  and that we can describe the temperature dependence of  $\xi$  and the relation between  $\omega_{sf}$  and  $\xi$  by Eqs.(12) and (13), respectively. Second, we assume that the hyperfine coupling constants are only weakly doping dependent, and that to good approximation we can use the same constants we extracted from the analysis of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ . Third, we need an estimate for  $T_{cr}$ , which is unknown for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ . However, since  $T_{cr} \approx 500 \text{ K}$  for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ , and since  $T_{cr}$  increases with decreasing doping, we assume  $T_{cr} \approx 550 - 650 \text{ K}$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ . To demonstrate the effect of the uncertainty in the latter assumption, we calculate the parameters  $\alpha, \omega_{sf}(T)$  and  $\xi(T)$  for  $T_{cr} = 650 \text{ K}$  and  $T_{cr} = 550 \text{ K}$  as well as for two different values of the momentum cut-off  $\Lambda$ . The resulting parameter sets based on experimental data by Takigawa *et al.* [26] are shown in Table I. Note that the parameters in Table I are rather robust against large variations in  $T_{cr}$  and/or  $\Lambda$  and only differ at the most by about 30%. In Fig. 4 we compare our theoretical results for the relaxation rates,  $1/T_1$  and  $1/T_{2G}$ , with the experimental data by Takigawa *et al.* [26]. We find that the temperature dependence of the relaxation rates calculated for each of the four different parameter sets in Table I, is practically indistinguishable; we therefore only plot the results for the parameter set with  $T_{cr} = 650 \text{ K}$  and  $\Lambda = 2\sqrt{\pi}$ . This result is consistent with the robustness of the scaling behavior in the commensurate case against non-universal lattice corrections as found for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ . We find a consistent description of the experimental data for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$  using the assumption of a  $z = 1$  scaling relationship and local commensuration in the temperature regime  $T_* \approx 230 \text{ K} < T < 300 \text{ K}$ , and, as was the case for  $\text{YBa}_2\text{Cu}_4\text{O}_8$ , assuming commensurate behavior leads to results which are practically independent of non-universal lattice corrections.

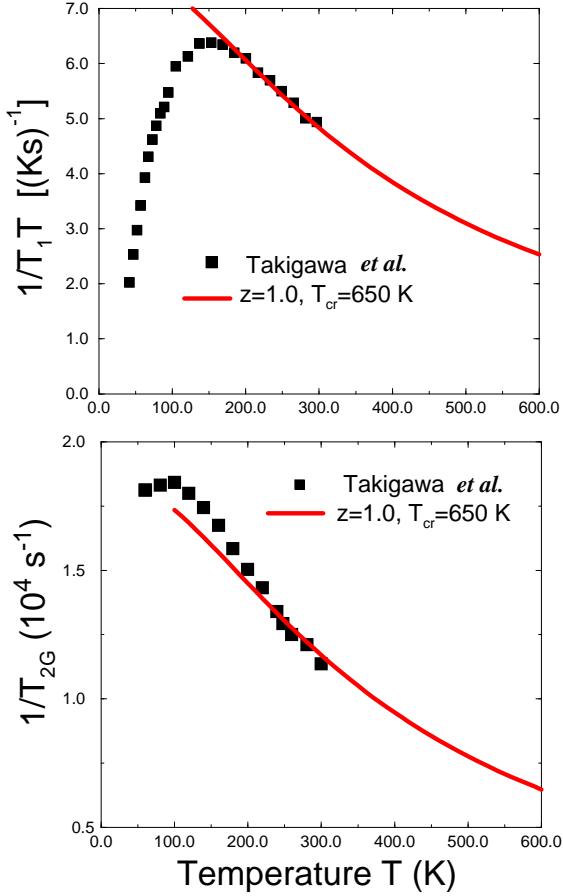


FIG. 4. Comparison of our theoretical results for the temperature dependence of  $1/T_1T$  (upper figure), and  $1/T_{2G}$  (lower figure) in  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$  with the experimental data by Takigawa *et al.* [26].

#### IV. INELASTIC NEUTRON SCATTERING

In this section we address the following two questions: (i) What is the effect of lattice corrections on the local susceptibility, and (ii) can one describe the available INS data with the parameter set extracted in the previous section?

As we discussed in the introduction we expect lattice corrections to lead to substantial corrections of  $\chi''_{loc}$  at frequencies larger than  $\omega_{sf}$ . Above this energy scale we also expect that the typical energy,  $\Delta_{sw}$ , of propagating spin waves, which, at low frequencies are completely overdamped by particle hole excitations, comes into play, leading to a modified form of the spin susceptibility

$$\chi(\mathbf{q}, \omega) = \frac{\alpha \xi^2}{1 + \xi^2(\mathbf{q} - \mathbf{Q})^2 - i\omega/\omega_{sf} - (\omega/\Delta_{sw})^2}. \quad (14)$$

For  $\omega < \Delta_{sw}^2/\omega_{sf}$  no sign of a propagating peak exists due to the diffusive character of the spin excitations. For  $\omega > \Delta_{sw}^2/\omega_{sf}$  and  $\mathbf{q} = \mathbf{Q}$  the consequence of a propa-

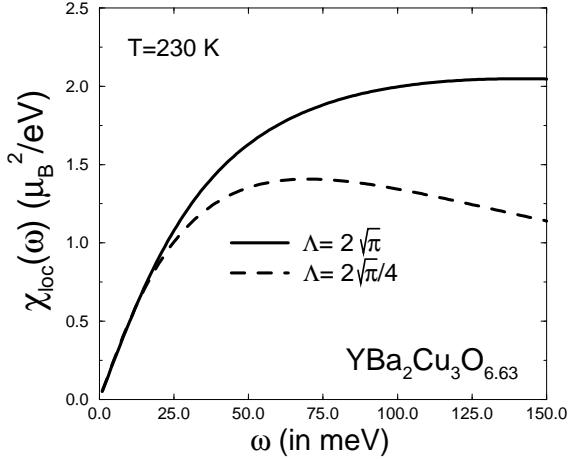


FIG. 5. The local susceptibility  $\chi''_{loc}(\omega)$  as a function of frequency for two different values of  $\Lambda$ .

gating mode is a pronounced pole in the excitation spectrum if  $\Delta_{sw} < \omega_{sf}$  and a soft upper cut off in energy if  $\Delta_{sw} > \omega_{sf}$ . The form of  $\chi(\mathbf{q}, \omega)$  in Eq.(14) can be shown to describe the propagating spin mode in  $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$  above  $T_c$  [27].

Using the parameter sets (1) and (2) in Table I, extracted in the previous section from NMR experiments, we plot in Fig. 5 the local susceptibility of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$  for two different values of  $\Lambda$ . We clearly see that upon decreasing the momentum cut-off, the maximum in  $\chi''_{loc}$  moves towards lower frequencies. Experimentally, however, the intensity at higher frequencies drops much faster than in Fig. 5, even for  $\Lambda = 2\sqrt{\pi}/4$  [28]. In order to explain this discrepancy, we note that at higher frequencies, the dominant contribution to  $\chi''_{loc}$  comes from regions in momentum space which are far away from the peak position at  $(\pi, \pi)$ . In these regions,  $\chi''(\mathbf{q}, \omega)$  is only weakly momentum dependent in which case its contribution might be easily attributed to the experimental background. In other words, we believe that the origin of the discrepancy lies in an underestimate of the experimental intensity at higher frequencies due to the problems one has in resolving it from the background [29].

In Fig. 6 we plot the calculated INS intensity, i.e.,  $\chi''(\mathbf{Q}, \omega)$  as a function of frequency at  $\mathbf{Q} = (\pi, \pi)$ . Since the calculated intensity is practically the same for all four parameter sets in Table I, we only present  $\chi''(\mathbf{Q}, \omega)$  calculated with the second parameter set in Table I (solid line). In the same figure, we also include the experimental data by Fong *et al.* for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.7}$  [30]. For the temperature range of interest, this material is the closest match for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ . Calculating the overall INS intensity with the parameters extracted from NMR experiments in the previous section, we find that we underestimate the experimental INS intensity by about 56 %, or a factor of 2.3 (the dashed line shows the calculated INS intensity, multiplied by an overall factor of 2.3). Given the uncer-

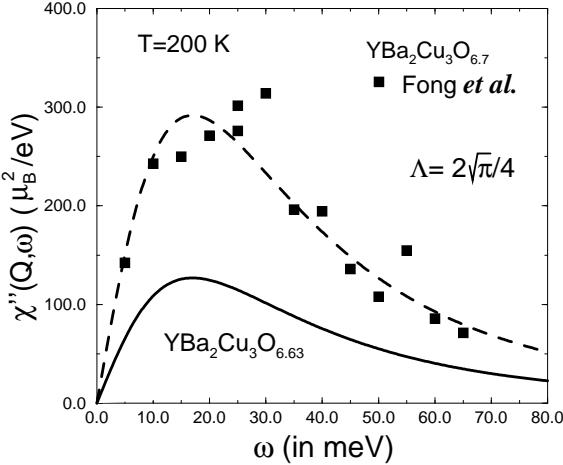


FIG. 6.  $\chi''(\mathbf{Q}, \omega)$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ . (a) Solid line:  $\chi''(\mathbf{Q}, \omega)$  calculated with parameter set (2) in Table I from NMR experiments. (b) Dashed line:  $\chi''(\mathbf{Q}, \omega)$  from (a) multiplied by an overall factor of 2.3. The experimental data are from Fong *et al.* [30].

tainties in the experimental determination of the absolute scale of  $\chi''$ , we believe that the above result represents reasonable agreement between the INS and NMR data and thus demonstrates consistency in the description of spin excitations based on these two experimental techniques.

## V. SPIN AND CHARGE INHOMOGENEITIES

We saw in Sec. III A that under the assumption of  $z = 1$  scaling, supported by recent INS experiments [15], a locally incommensurate magnetic response is inconsistent with the available experimental NMR data. We therefore concluded that NMR data support a locally commensurate magnetic structure. The question thus arises of how one can understand a locally commensurate, but globally incommensurate magnetic response as seen by INS? It has been suggested that charge stripes separated by an average distance  $l_0 = 2\pi/\delta$  are the origin of the incommensurate magnetic response seen in INS experiments [31]. For a large part of the sample this would leave the locally commensurate structure intact. Except for the Nd-doped 214 compounds [32] and probably for the particular doping value  $x = \frac{1}{8}$  in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_2$ , these stripes are believed to be dynamic rather than static in nature.

Considering a spatial charge variation:

$$\rho(r) = \rho_0 + \delta\rho(r), \quad (15)$$

where  $\rho_0$  is independent of  $r$ . The question arises whether the system is in a regime with  $\rho_0 \ll \delta\rho(r)$ , as suggested in Ref. [31], or rather characterized by rather small charge

variations, i.e.  $\delta\rho(r) < \rho_0$ . The particular appeal of the former assumption of strong charge modulations is an immediate explanation of the doping dependence of the position of the incommensurate peak,  $\delta = 2x$ . Stripes with one hole every second lattice site in a hole free antiferromagnetic environment move closer together upon doping, leading to the above  $x$ -dependence of  $\delta$ . Also, the exceptional behavior of various magnetic and transport properties for the doping value  $x = \frac{1}{8}$  can be easily understood in terms of a stable commensurate arrangement of such stripes and the underlying lattice. Another argument in favor of this scenario are the recent results by Vojta and Sachdev [33] who investigated the mean field behavior of a system with competing magnetic and long range Coulomb interactions and found areas with a strong charge modulation separated by regions with barely disturbed antiferromagnetic correlations.

Nevertheless, there are several conceptional problems with such a strong charge modulation, which lead us to present some arguments favoring a more moderate charge variation,  $\delta\rho(r) < \rho_0$ , under circumstances that the transverse mobility of the charge carriers with respect to the averaged position of the stripes is large. First, uncorrelated spatial stripes of width  $r_0$ , which fluctuate transversely over a distance  $d$ , will give rise to a broadening  $d/l_0^2$  of the magnetic peaks observed by INS. The experimental INS results, however, provide strong support for a scenario in which the width of the magnetic peaks is determined by  $\xi^{-1}$  [15]. Thus, in order to observe separated incommensurate peaks, we need at least  $\xi \gg d$  to establish a well defined antiphase domain wall, implying  $d \ll l_0$ . In other words, assuming uncorrelated stripes, the width  $d$  over which stripes fluctuate must be very small to account for the existing INS data. Such "stiff" but uncorrelated stripes seem to be in contradiction to the notion of stripes as a dynamical entity. Therefore, we arrive at the conclusion that spatial stripe fluctuations, if they exist, must be strongly correlated.

Second, at the characteristic temperatures where stripes with  $\rho_0 \ll \delta\rho(r)$  appear, strong modifications of the resistivity and other transport properties are expected to occur. None or only moderate changes of this kind have been observed and no indication for a dimensional crossover from quasi one-dimensional to quasi two-dimensional dynamics seems to be present.

Third, for low frequencies, the spin excitations in doped cuprates are overdamped rather than propagating spin waves. The suppression of the spin damping upon opening of a quasiparticle gap in the superconducting as well as in the pseudogap state implies that the dominant source of the spin damping,  $\gamma$ , are particle-hole excitations. Assuming weak charge modulations, we then find  $\text{Im}\chi^{-1}(\omega) \propto \gamma\omega$ , in agreement with the results of INS experiments [15].

On the other hand, rigid stripes separated by one dimensional charge carriers, which are effectively bosonic in character, lead to strong deviations from the above frequency dependence of  $\text{Im}\chi^{-1}(\omega)$  [34,35], in disagree-

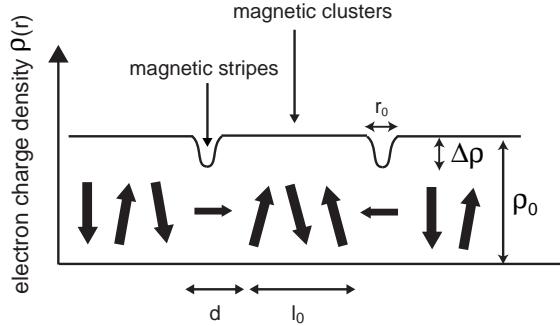


FIG. 7. Schematic picture of charge and spin inhomogeneities.

ment with INS experiments. Thus,  $\text{Im}\chi^{-1}(\omega)$  does not arise from spatially varying stripes even though they certainly affect the spin degrees of freedom and can cause the decay of these excitations.

Finally, NMR and other magnetic measurements on various cuprates which provide strong support for spatial inhomogeneities [36–41] suggest mostly spatially varying *spin* degrees of freedom but not necessarily a strong modulation of the charge background.

The above points suggest that the inhomogeneities observed in the high- $T_c$  cuprates might be predominantly magnetic in origin with only moderate modulations of the charge density. This is not unrealistic since in strongly correlated systems small variations in the charge density can bring about substantial changes in the magnetic properties of the system. This scenario of a predominantly magnetic character of the inhomogeneities, leading to magnetic stripes and clusters, is schematically presented in Fig. 7. Note, that the magnetic stripes, in which the electronic charge density is lower than that in the magnetic clusters, represent magnetic domain walls with a phase slip of  $\pi$  in the ordering of the spins. Theoretically, we believe that this more homogeneous charge arrangement is a result of quantum fluctuations beyond the mean field level investigated in Ref. [33].

The formation of magnetic clusters and stripes requires competing interactions on different length scales. Besides the local Coulomb interaction, we need to identify a longer length scale interaction. It was argued earlier that in the cuprate superconductors an increase of the magnetic correlation length leads to strong vertex corrections, which in turn give rise to a gradient coupling between the fermionic and spin degrees of freedom [42]. For a system with an ordered ground state, this takes the form of a dipole-dipole coupling which has been shown to cause inhomogeneities and domain formation in two dimensional magnetic systems. The length scale of this gradient coupling should roughly speaking be the magnetic correlation length,  $\xi$ . We thus need a minimum value of  $\xi$  to (a) generate the gradient coupling, and to (b) observe the incommensuration. The temperature at

which incommensuration should appear is roughly set by  $\xi(T) \approx l_0 = 4$ , where the last equality arises from the momentum position of the incommensurate peaks. Since, as we argued earlier,  $\xi(T_{cr}) \approx 2$ ,  $T_{cr}$  thus presents an upper bound for the formation of magnetic clusters. This anomalous coupling is of course enhanced once magnetic clusters are formed; the creation of magnetic inhomogeneities is a self-consistent process. The magnetic inhomogeneity scenario presented here is admittedly very qualitative and further microscopic investigations will be required to verify or disprove it.

## VI. CONCLUSIONS

In this communication, we investigated whether it is possible to understand theoretically INS and NMR data within a single theoretical framework. Based on the observation of an incommensurate structure of the magnetic response by INS experiments [8,15], we considered whether this reflects a locally or globally incommensurate ordering. On analyzing NMR data on  $\text{YBa}_2\text{Cu}_4\text{O}_8$  we found with the condition of  $z = 1$  scaling that a homogeneous incommensuration is, within the framework given by Eq.(1), inconsistent with the available experimental data. We thus concluded that the local magnetic structure as probed by NMR is likely commensurate.

We then investigated the effect of lattice corrections on both the parameter sets extracted from NMR data and on the local susceptibility measured in INS experiments. We found that while the resulting corrections to the NMR parameters are only weak, the most pronounced effect of such corrections appears in the local susceptibility determined in INS measurements at frequencies above  $\omega_{sf}$ . Specifically, we found that decreasing the momentum cut-off leads to a suppression of  $\chi''_{loc}$  at higher frequencies, thus improving the agreement with the experimental data. We argued that the remaining discrepancies can be explained by an experimental underestimate of the INS intensity at higher frequencies. Furthermore, we quantitatively compared INS and NMR data and found agreement within a factor of 2. Given the large uncertainties in resolving  $\chi''$  from the large background and in determining the absolute intensity of  $\chi''$ , we believe that this result demonstrates that a consistent description of INS and NMR data can be obtained using the expression for  $\chi$  given in Eq.(1).

Finally, we discussed a spin and charge inhomogeneity scenario to reconcile the local commensurations, as seen in NMR experiments, and the incommensurate peaks, seen by INS. This scenario, even though similar in spirit to earlier charge stripe pictures, is based on a moderate to weak modulation of the charge density, causing a pronounced inhomogeneity in the magnetic properties and leading to magnetically coupled clusters separated by weakly correlated stripes.

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